Matrices and Symmetry

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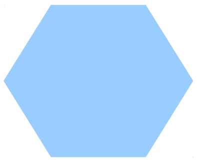
Mathematical background

An **object** is invariant upon a strictly defined **operation**

Clock **24 time**



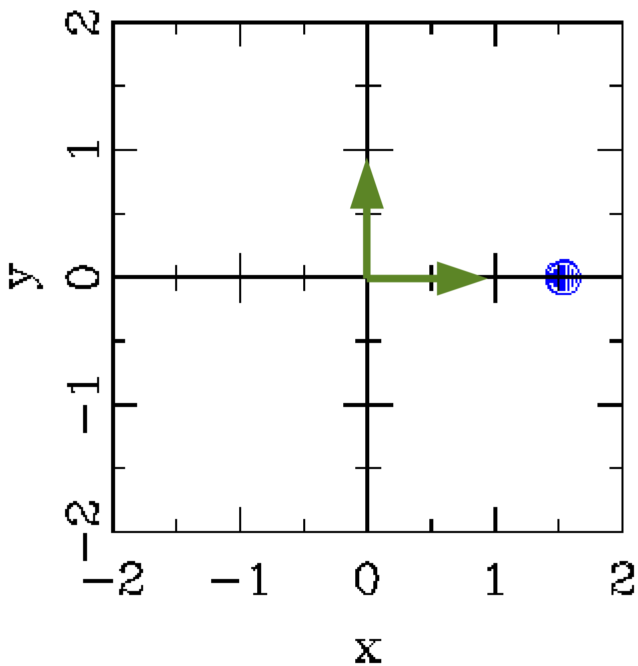
Rotation by 60°

Around axis normal to hexagon through central point

Within a crystal:

Rotation by	**360°, 1**	**180°, 2**	**120°, 3**	**90°, 4**	**60° 6**
Mirror plane		**m**			
Inversion	$\bar{1}$				
Rotoinversion	$\bar{1}$,	$\bar{2}$ = m	$\bar{3}$,	$\bar{4}$,	$\bar{6}$ = 3/m
Glide plane	**a, b, c,**	**n, d**			
Screw axis	M_N				
Translation	[1,0,0]	[0,1,0]	[0,0,1]		
	[½,½, 0]	[½, 0, ½]	[0, ½, ½]		
	[½, ½, ½]				
	[1/3, 2/3, 1/3]		[2/3, 1/3, 1/3]		

Copy one atom to new position



Requires more than descriptive words!

Need to define: **coordinate system**

Atom position

Symmetry operation

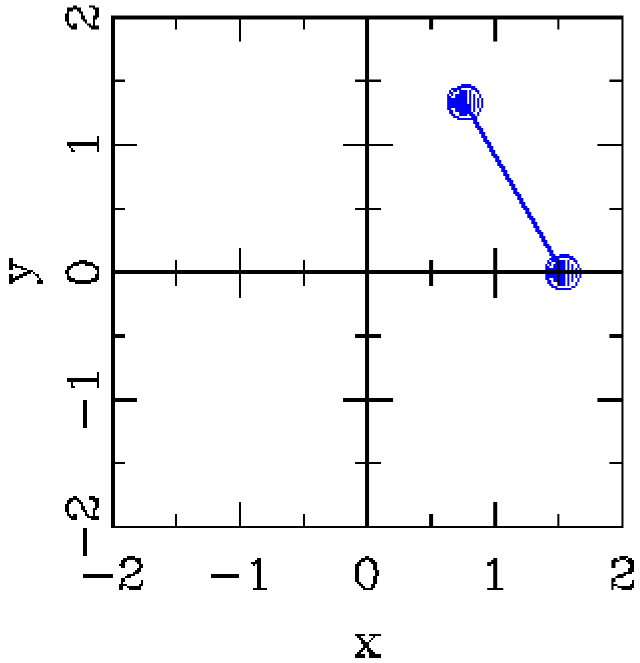
$$\begin{pmatrix}1.54\\0.00\\0.00\end{pmatrix} = 1.54\cdot\vec{a} + 0.00\cdot\vec{b} + 0.00\cdot\vec{c}$$

$$|\vec{a}| = |\vec{b}| = |\vec{c}| = 1.00$$

$$\alpha = \beta = \gamma = 90.00\,°$$

$$\begin{pmatrix}1.54\\0.00\\0.00\end{pmatrix}$$

Copy one atom to new position



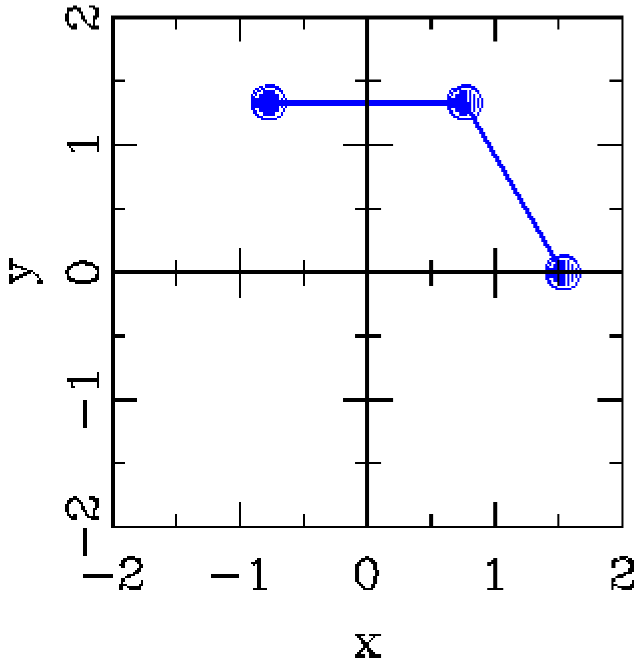
Need to define: coordinate system

Atom position

Rotate by 60°, counterclockwise
Around axis [0,0,1]

$$\begin{pmatrix}1.54\\0.00\\0.00\end{pmatrix} \rightarrow \begin{pmatrix}0.77\\1.33\\0.00\end{pmatrix}$$

Copy one **atom** to new position



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$$\begin{pmatrix} 1.54 \\ 0.00 \\ 0.00 \end{pmatrix} \rightarrow \begin{pmatrix} 0.77 \\ 1.33 \\ 0.00 \end{pmatrix} \rightarrow \begin{pmatrix} -0.77 \\ 1.33 \\ 0.00 \end{pmatrix}$$

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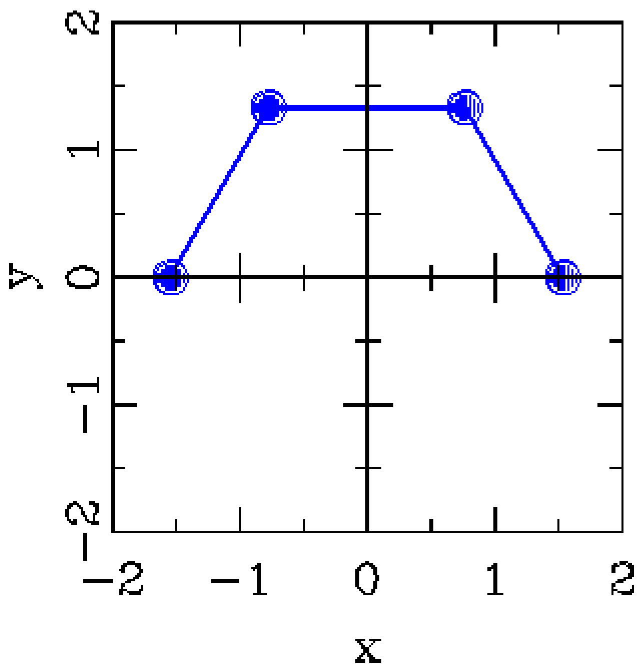

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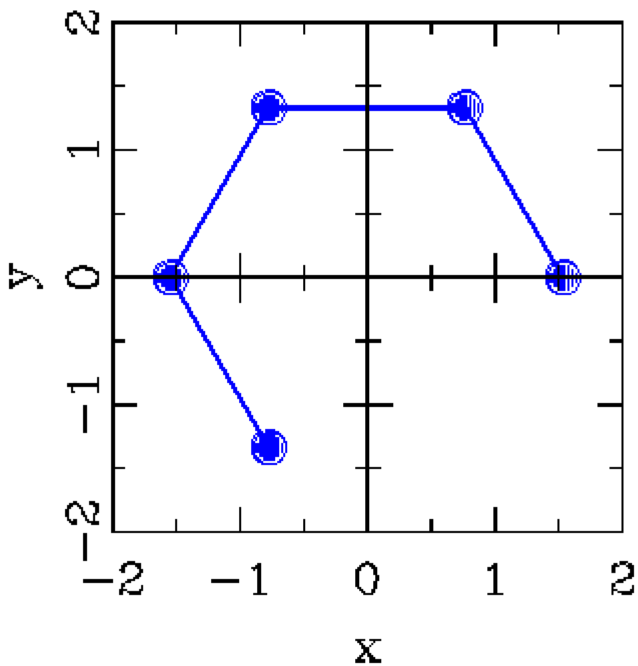

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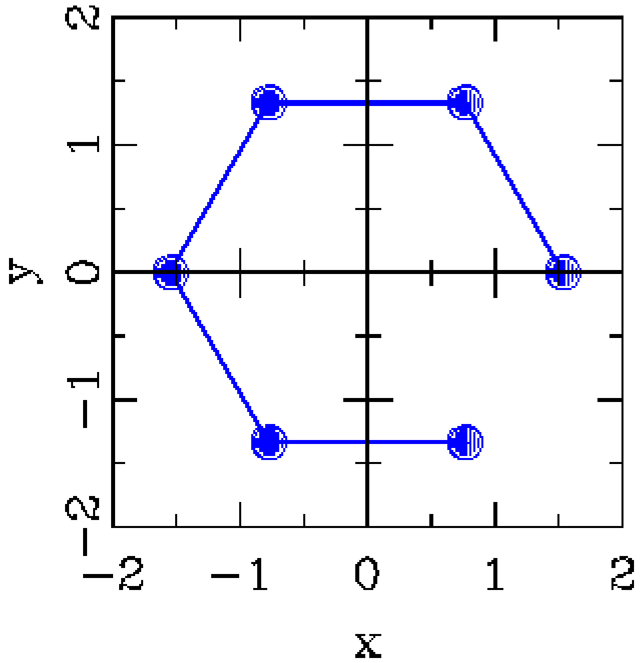
Copy one **atom** to new position



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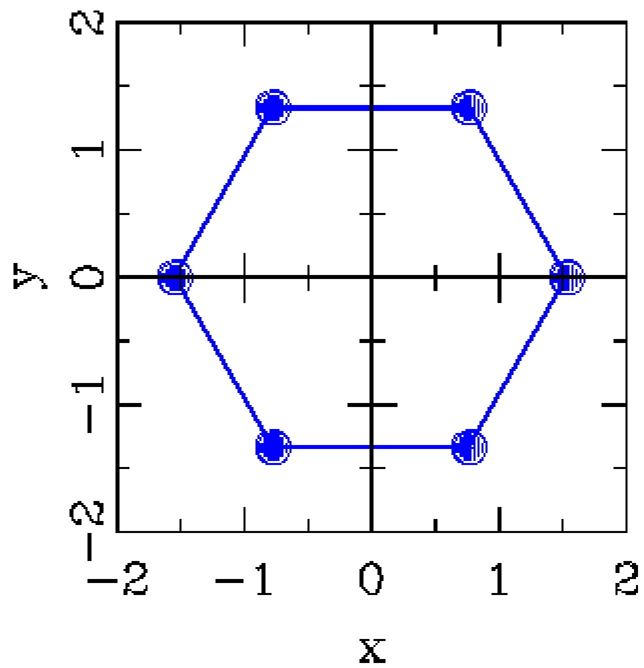

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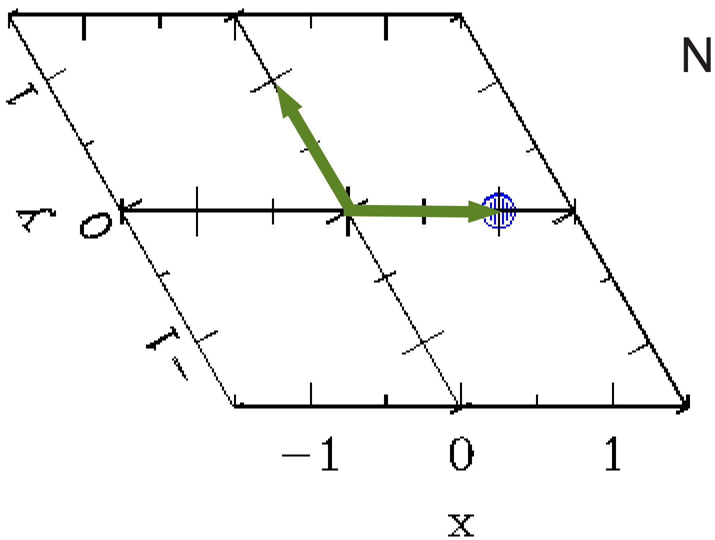


Need to define: **coordinate system**

Atom position

Rotate by 60°, counterclockwise
Around axis [0,0,1]

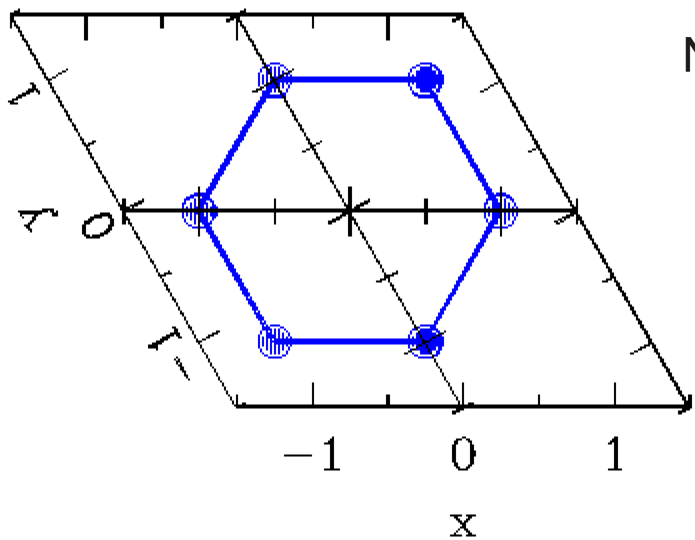
$$\begin{pmatrix}1.00\\0.00\\0.00\end{pmatrix} = 1.00\cdot\vec{a} + 0.00\cdot\vec{b} + 0.00\cdot\vec{c}$$

$$|\vec{a}| = |\vec{b}| = 1.54 \neq |\vec{c}|$$

$$\alpha = \beta = 90.00° \neq \gamma = 120°$$

$$\begin{pmatrix}1.00\\0.00\\0.00\end{pmatrix}$$

Copy one atom to new position



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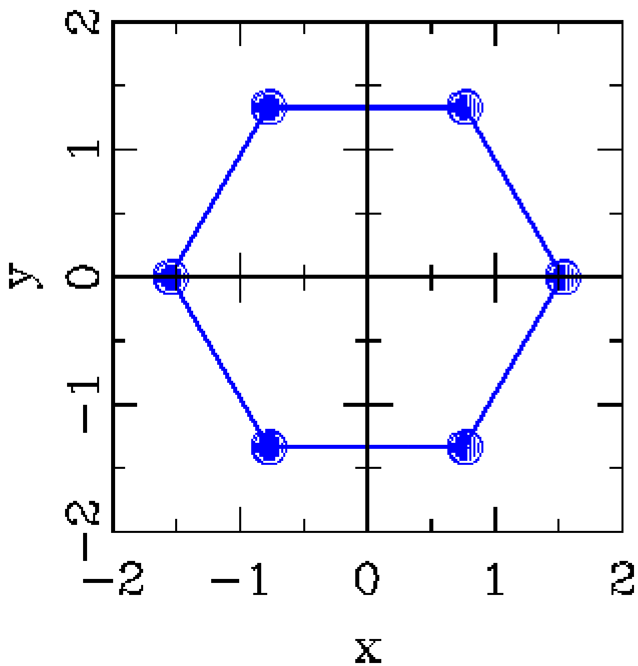
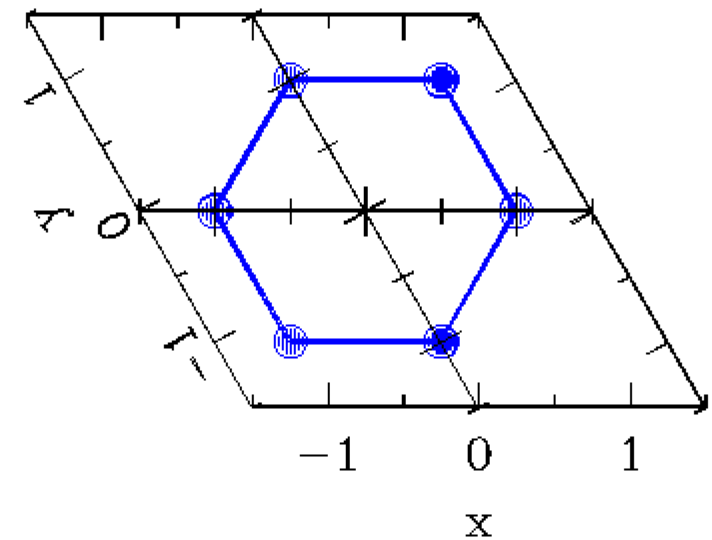
Rotate by 60°, counterclockwise
Around axis [0,0,1]

$$\begin{pmatrix}1.00\\0.00\\0.00\end{pmatrix} \rightarrow \begin{pmatrix}1.00\\1.00\\0.00\end{pmatrix} \rightarrow \begin{pmatrix}0.00\\1.00\\0.00\end{pmatrix} \rightarrow \begin{pmatrix}-1.00\\0.00\\0.00\end{pmatrix} \rightarrow \begin{pmatrix}-1.00\\-1.00\\0.00\end{pmatrix} \rightarrow \begin{pmatrix}0.00\\-1.00\\0.00\end{pmatrix}$$





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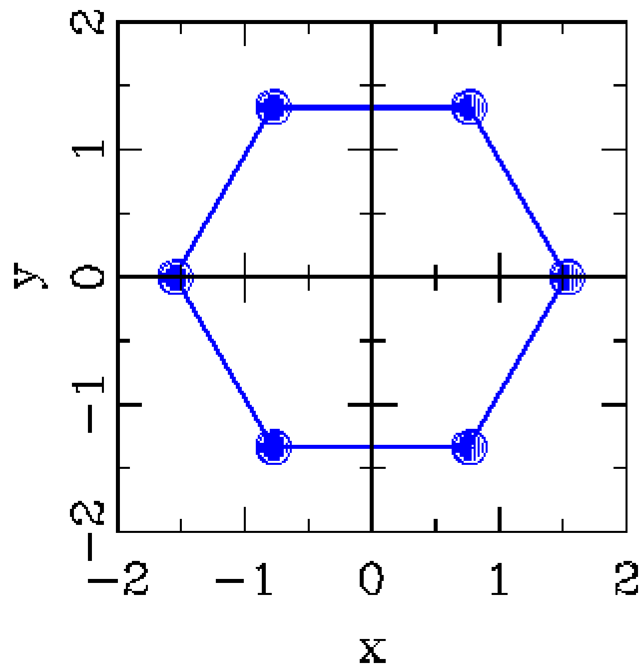
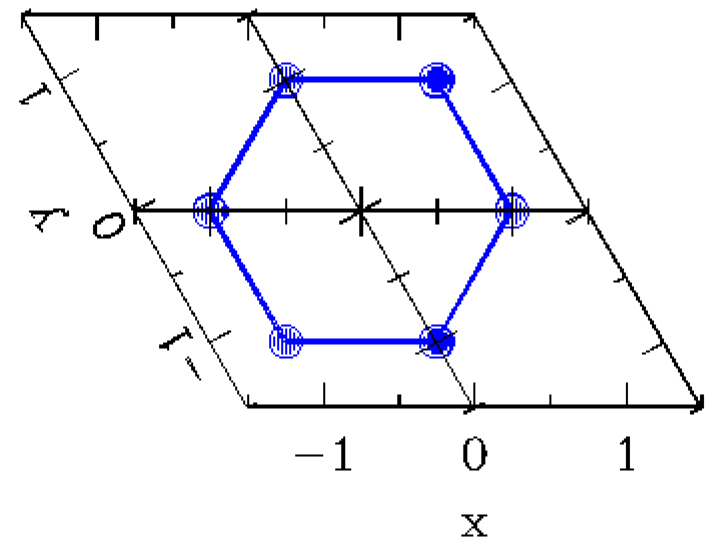
$$|\vec{a}| = |\vec{b}| = 1.54 \neq |\vec{c}|$$

$$\alpha = \beta = 90.00^\circ \neq \gamma = 120^\circ$$

Choice of coordinate system affects atom coordinates
Usually: Choose coordinate system that matches crystal symmetry





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Symmetry operations are special class of general transformations

- **Image** is indistinguishable from source
- **distances, angles** are **invariant** under **symmetry operation**

Symmetry operations are special class of general transformations

Image is indistinguishable from source

distances, angles are **invariant** under **symmetry operation**

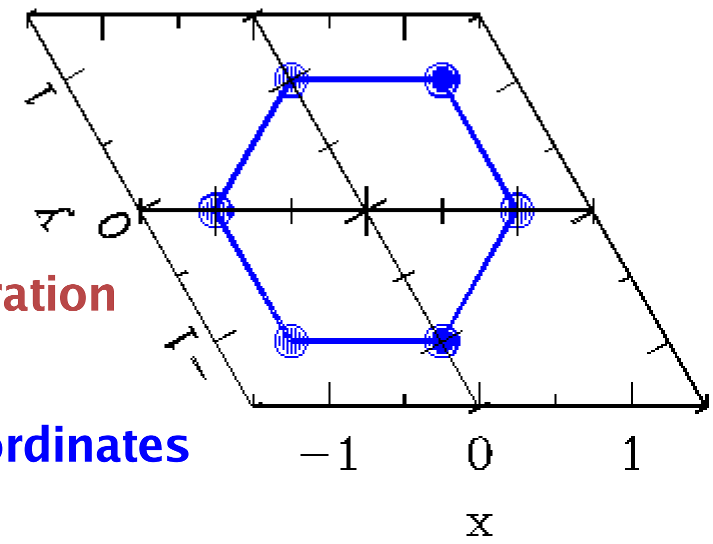
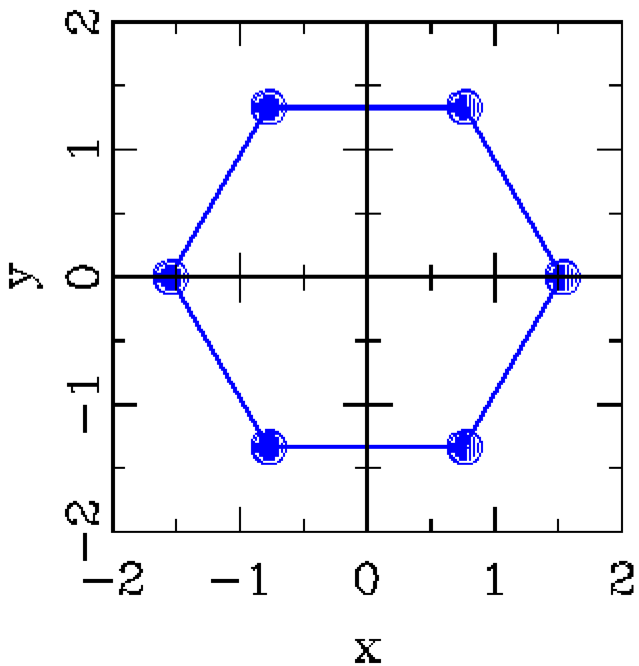


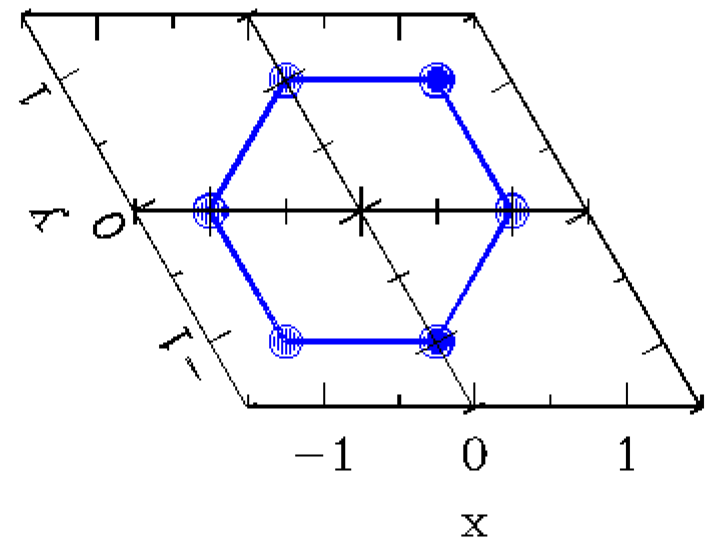
Image coordinates are **linear function** of **original coordinates**

$$x' = A_{11}x + A_{12}y + A_{13}z + t_1$$
$$y' = A_{21}x + A_{22}y + A_{23}z + t_2$$
$$z' = A_{31}x + A_{32}y + A_{33}z + t_3$$

$$\begin{pmatrix} 1.00 \\ 0.00 \\ 0.00 \end{pmatrix} \begin{pmatrix} 1.00 \\ 1.00 \\ 0.00 \end{pmatrix} \begin{pmatrix} 0.00 \\ 1.00 \\ 0.00 \end{pmatrix} \begin{pmatrix} -1.00 \\ 0.00 \\ 0.00 \end{pmatrix} \begin{pmatrix} -1.00 \\ -1.00 \\ 0.00 \end{pmatrix} \begin{pmatrix} 0.00 \\ -1.00 \\ 0.00 \end{pmatrix}$$

Symmetry as set of linear equations





$$\begin{pmatrix}1.54\\0.00\\0.00\end{pmatrix}\begin{pmatrix}0.77\\1.33\\0.00\end{pmatrix}\begin{pmatrix}-0.77\\1.33\\0.00\end{pmatrix}\begin{pmatrix}-1.54\\0.00\\0.00\end{pmatrix}\begin{pmatrix}-0.77\\-1.33\\0.00\end{pmatrix}\begin{pmatrix}0.77\\-1.33\\0.00\end{pmatrix}$$

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$$\begin{aligned}x' &= 0.500\,x - 0.866\,y + 0.000\,z + 0.000\\ y' &= 0.866\,x + 0.500\,y + 0.000\,z + 0.000\\ z' &= 0.000\,x + 0.000\,y + 1.000\,z + 0.000\end{aligned}$$

$$\begin{aligned}x' &= 1\,x - 1\,y + 0\,z + 0.000\\ y' &= 1\,x + 0\,y + 0\,z + 0.000\\ z' &= 0\,x + 0\,y + 1\,z + 0.000\end{aligned}$$

Image coordinates are **linear function** of **original coordinates**

$$x' = A_{11}x + A_{12}y + A_{13}z + t_1$$
$$y' = A_{21}x + A_{22}y + A_{23}z + t_2$$
$$z' = A_{31}x + A_{32}y + A_{33}z + t_3$$

Take **image coordinates**, **input coordinates** and **t** as (3x1)= column vectors

Take coefficients A_{ij} as (3x3)= matrix

And use multiplication rules to get

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} * \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix} \qquad \vec{x}' = \underline{\underline{A}} \cdot \vec{x} + \vec{t}$$

$$\begin{pmatrix} \boxed{x'} \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \boxed{A_{11} \quad A_{12} \quad A_{13}} \\ A_{21} \quad A_{22} \quad A_{23} \\ A_{31} \quad A_{32} \quad A_{33} \end{pmatrix} * \boxed{\begin{pmatrix} x \\ y \\ z \end{pmatrix}} + \begin{pmatrix} \boxed{t_1} \\ t_2 \\ t_3 \end{pmatrix}$$

Multiply row by column

Rank: Number of indices — Ranks must be identical

Dimension: largest value of an index = number of rows or number of columns

(M x N) M Rows and N columns

(**M** x **N**) = (**M** x K) (K x **N**) Number of columns = number of rows

(**4** x **2**) (**4** x 3) (3 x **2**)

$$\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \\ C_{31} & C_{32} \\ C_{41} & C_{42} \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \\ A_{41} & A_{42} & A_{43} \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \\ B_{31} & B_{32} \end{pmatrix}$$

Rows from 1st
Columns from 2nd

Number of columns = number of rows

$$C_{I\,L} = \sum_{K=1}^{K_{dim}} A_{I\,K} \cdot B_{K\,L}$$

For us almost always

(**3** x **1**) = (**3** x 3)(3 x **1**)

(**3** x **3**) = (**3** x 3)(3 x **3**)

$$\underline{\underline{A}}\,\underline{\underline{B}} \neq \underline{\underline{B}}\,\underline{\underline{A}}$$

Determinant of a matrix:

$$\det\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} = A_{11}(A_{22}A_{33}-A_{32}A_{23}) - A_{12}(A_{21}A_{33}-A_{31}A_{23}) + A_{13}(A_{21}A_{32}-A_{31}A_{22})$$

$$\det\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} = \begin{pmatrix} \boxed{\mathbf{A_{11}}} & A_{12} & A_{13} \\ A_{21} & \mathbf{A_{22}} & \mathbf{A_{23}} \\ A_{31} & \mathbf{A_{32}} & \mathbf{A_{33}} \end{pmatrix} - \begin{pmatrix} A_{11} & \boxed{\mathbf{A_{12}}} & A_{13} \\ \mathbf{A_{21}} & A_{22} & \mathbf{A_{23}} \\ \mathbf{A_{31}} & A_{32} & \mathbf{A_{33}} \end{pmatrix} + \begin{pmatrix} A_{11} & A_{12} & \boxed{\mathbf{A_{13}}} \\ \mathbf{A_{21}} & \mathbf{A_{22}} & A_{23} \\ \mathbf{A_{31}} & \mathbf{A_{32}} & A_{33} \end{pmatrix}$$

Symmetry operations: Rotations, Identity det(S) = +1

Mirror, Inversion, Rotoinversion det(S) = -1

Trace = sum of diagonal element

Addition: (4 x 2) = (4 x 2) + (4 x 2)

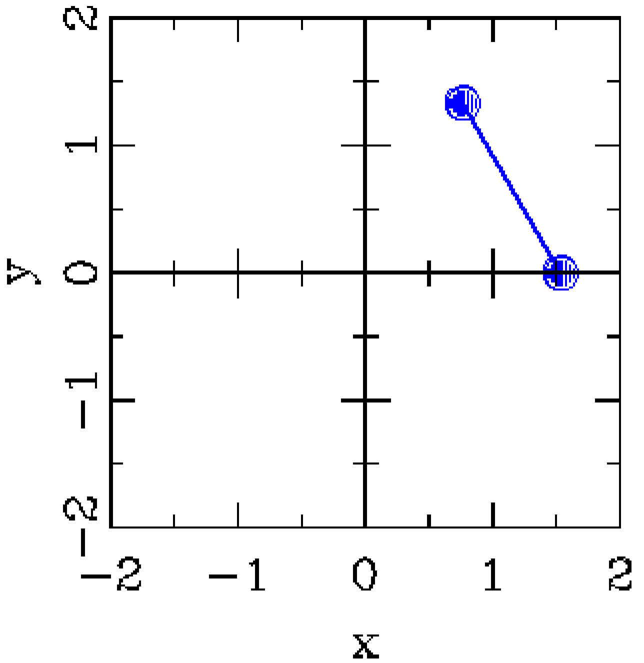
Ranks identical
All dimensions identical

$$C_{IL} = A_{IL} + B_{IL}$$

Cartesian Space

Rotation around z axis by angle α

$$\begin{pmatrix} \cos(\alpha) & -\sin(\alpha) & 0 \\ \sin(\alpha) & \cos(\alpha) & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$



Determinant is +1

Trace = $2\cos(\alpha) + 1$

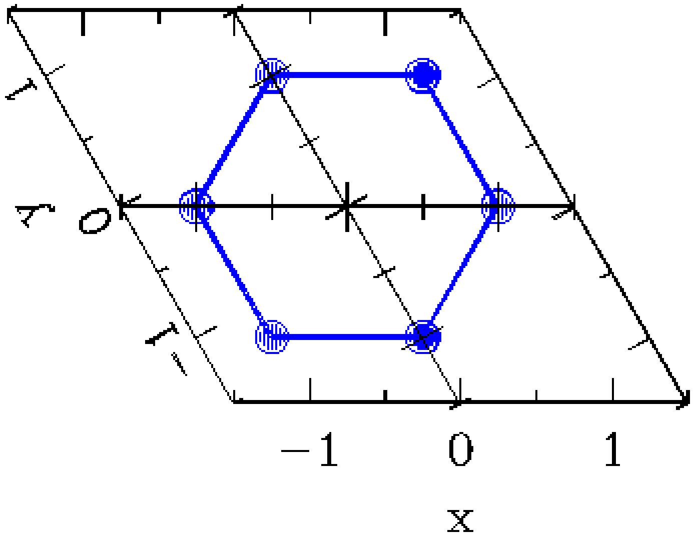
α	cos(α)	Tr
180°	-1	-1
120°	-0.5	0
90°	0	1
60°	0.5	2
0°	1	3

$$\begin{pmatrix} 1.54 \\ 0.00 \\ 0.00 \end{pmatrix} \rightarrow \begin{pmatrix} 0.77 \\ 1.33 \\ 0.00 \end{pmatrix}$$

Hexagonal Space

Rotation around z axis by angle α

$$\begin{pmatrix} 1 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$



$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \Rightarrow \begin{pmatrix} x-y \\ x \\ z \end{pmatrix}$$

All rotation matrices in crystal space have elements {-1, 0, 1}

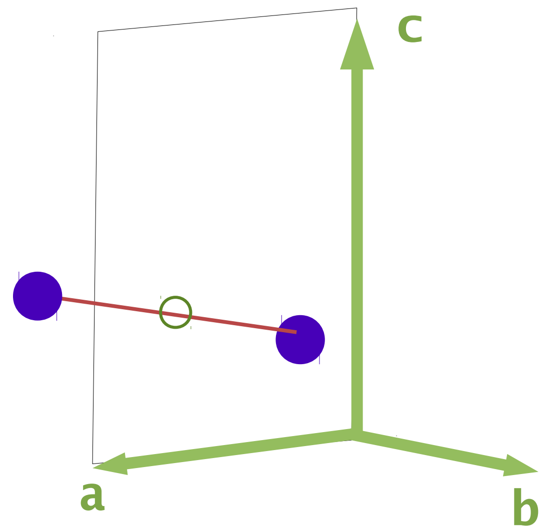
Determinant is +1

Trace = +2

Monoclinic Space

Mirror on x0z plane

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$



$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \Rightarrow \begin{pmatrix} x \\ -y \\ z \end{pmatrix}$$

All mirror matrices in crystal space have elements {-1, 0, 1}

Determinant is -1

Trace = +1

Any Space

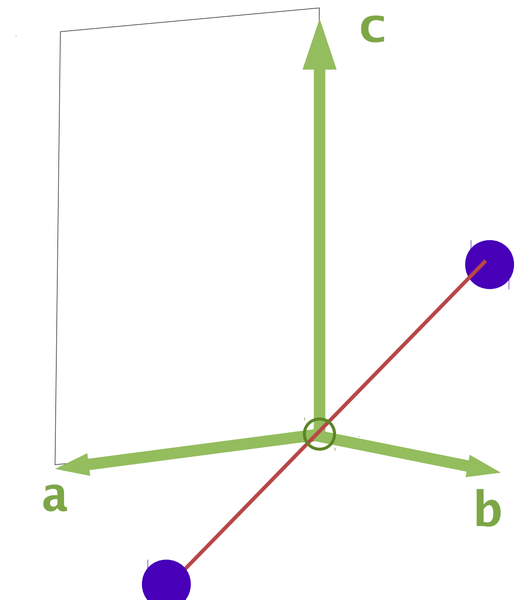
Inversion

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

Unit matrix multiplied by -1

Determinant is -1

Trace = -3

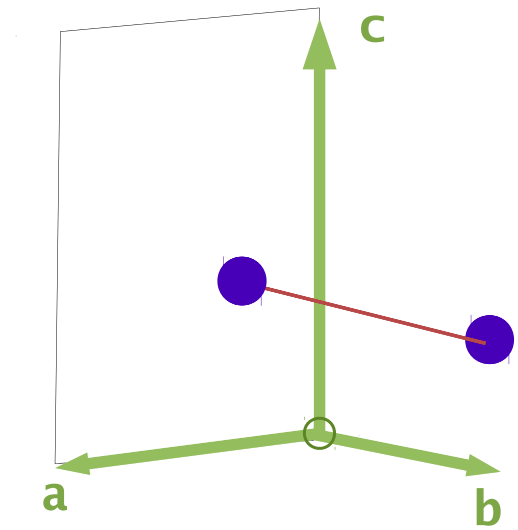


$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \rightarrow \begin{pmatrix} -x \\ -y \\ -z \end{pmatrix}$$

Any Space

Translation

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix}$$



Unit matrix plus translation vector

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \Rightarrow \begin{pmatrix} x + t_1 \\ y + t_2 \\ z + t_3 \end{pmatrix}$$

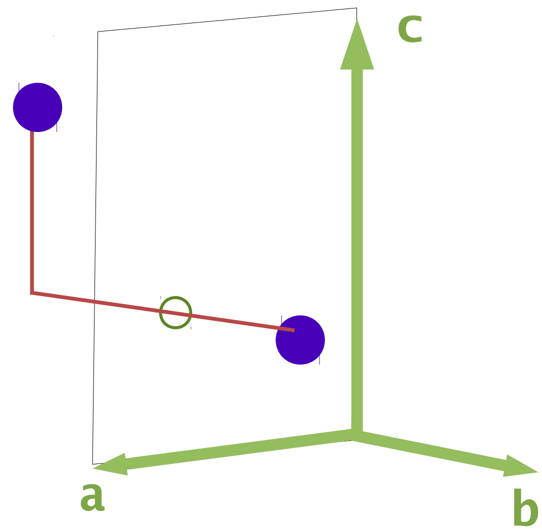
Determinant is 1

Trace = 3

Monoclinic Space

c-glide plane on x0z plane

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 1/2 \end{pmatrix}$$



Combination of mirror matrix
plus translation parallel c

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \Rightarrow \begin{pmatrix} x \\ -y \\ z + 1/2 \end{pmatrix}$$

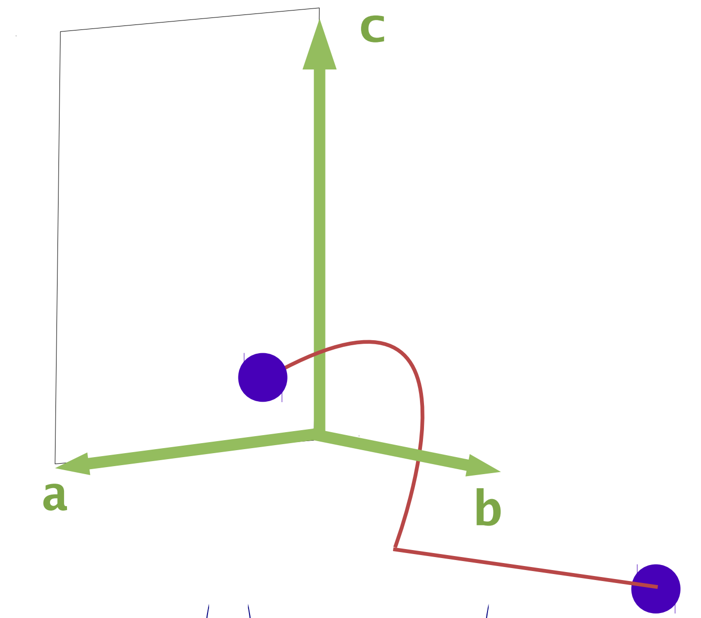
Determinant is -1

Trace = +1

Monoclinic Space

2_1 screw axis parallel to [0y0]

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 1/2 \\ 0 \end{pmatrix}$$



$$\begin{pmatrix} x \\ y \\ z \end{pmatrix} \Rightarrow \begin{pmatrix} -x \\ y + 1/2 \\ -z \end{pmatrix}$$

Combination of rotation matrix
plus translation parallel b

Determinant is +1

Trace = -1

Consecutive application of two(any) symmetry operations

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \left[\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} * \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix} \right]$$

$$\begin{pmatrix} x'' \\ y'' \\ z'' \end{pmatrix} = \begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix} * \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} + \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}$$

$$\begin{pmatrix} x'' \\ y'' \\ z'' \end{pmatrix} = \begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix} * \left[\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} * \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix} \right] + \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}$$

$$\begin{pmatrix} x'' \\ y'' \\ z'' \end{pmatrix} = \begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix} * \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} * \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} B_{11} & B_{12} & B_{13} \\ B_{21} & B_{22} & B_{23} \\ B_{31} & B_{32} & B_{33} \end{pmatrix} \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix} + \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}$$

$$\begin{pmatrix} x'' \\ y'' \\ z'' \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{pmatrix} * \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}$$

Consecutive application of two(any) symmetry operations

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \left[\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} * \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix} \right]$$

$$\vec{x}'' = \underline{\underline{B}} \cdot \vec{x}' + \vec{u} \longleftarrow \vec{x}' = \underline{\underline{A}} \cdot \vec{x} + \vec{t}$$

$$\vec{x}'' = \underline{\underline{C}} \cdot \vec{x} + \vec{w}$$

with: $\underline{\underline{C}} = \underline{\underline{B}} \cdot \underline{\underline{A}}$ and: $\vec{w} = \underline{\underline{B}} \cdot \vec{t} + \vec{u}$

$\{\underline{\underline{A}}, \vec{t}\}$

$\{\underline{\underline{W}}, \vec{w}\}$

Notation in Int. Tables

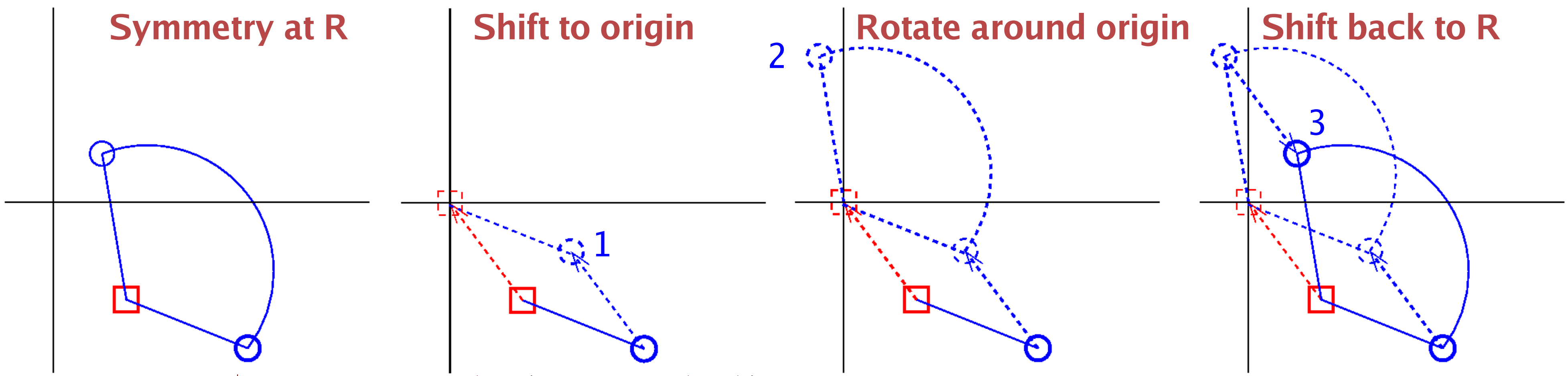
Augmented form

$$\begin{pmatrix} x' \\ y' \\ z' \\ 1 \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} & t_1 \\ A_{21} & A_{22} & A_{23} & t_2 \\ A_{31} & A_{32} & A_{33} & t_3 \\ 0 & 0 & 0 & 1 \end{pmatrix} * \begin{pmatrix} x \\ y \\ z \\ 1 \end{pmatrix}$$

$$\ddot{\vec{x}}'' = \underline{\underline{\tilde{B}}} \cdot \ddot{\vec{x}} \longleftarrow \ddot{\vec{x}}' = \underline{\underline{\tilde{A}}} \cdot \ddot{\vec{x}}$$

$$\ddot{\vec{x}}'' = \underline{\underline{\tilde{C}}} \cdot \ddot{\vec{x}}$$

then: $\underline{\underline{\tilde{C}}} = \underline{\underline{\tilde{B}}} \cdot \underline{\underline{\tilde{A}}}$



$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} * \left[\begin{pmatrix} x \\ y \\ z \end{pmatrix} - \begin{pmatrix} R_x \\ R_y \\ R_z \end{pmatrix} \right] + \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix} + \begin{pmatrix} R_x \\ R_y \\ R_z \end{pmatrix}$$

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} * \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix} + \left[\begin{pmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{pmatrix} - \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right] \begin{pmatrix} R_x \\ R_y \\ R_z \end{pmatrix}$$

$$\vec{x}' = \underline{\underline{A}} \cdot \left[\vec{x} - \vec{R} \right] + \vec{t} + \vec{R}$$

$$\vec{x}' = \underline{\underline{A}} \cdot \vec{x} + \vec{t} + \left[\underline{\underline{A}} - \underline{\underline{I}} \right] \cdot \vec{R}$$

Additional translation, independent of x

$$\vec{x}' = \underline{\underline{A}} \cdot \vec{x} + \vec{t}'$$

Requires good documentation

Space group C 2/c no 15

Origin at $\bar{1}$ on glide c

Symmetry operations

For (0,0,0)+ set   Normal symmetry operations

(1) 1   (2) 2 0, y, ¼   (3) $\bar{1}$ 0, 0, 0   (4) c x, 0, z

For (½, ½, 0)+ set   symmetry operations that include the C-centering

(1) t(½, ½, 0)   (2) 2(0, ½, 0) ¼, y, ¼   (3) $\bar{1}$ ¼, ¼, 0   (4) n(½, 0, ½) x, ¼, z

Names:	(No)	type	(translation component)	location
			if present, and NOT Obvious by name	describes points that are on the rotation axis or mirror plane
For $\bar{N}$:	(No)	$\bar{N}$	location; location	
In $Fm\bar{3}m$	(41)	$\bar{4}$-	x,0,0; 0,0,0 axis; inversion center	

Symmetry in the International Tables Vol. A

Generators (1); t(1,0,0); t(0,1,0); t(0,0,1); t(½, ½, 0); (2); (3)

Positions | Coordinates

Multiplicity
Wyckoff letter
Site symmetry

(0,0,0)+ (½ , ½ , 0)+ Add these vectors to ALL atom positions listed

8 f 1 (1) x, y, z (2) $\bar{x}$, y, $\bar{z}$ + ½ (3) $\bar{x}$, $\bar{y}$, $\bar{z}$ (4) x, $\bar{y}$, z + ½

8 = No of atom positions

(2) $\bar{x}$, y, $\bar{z}$ + ½ (Number) identical to list on previous page

$$\begin{pmatrix} -x \\ y \\ -z+1/2 \end{pmatrix}_2 \xleftarrow{(2)} \begin{pmatrix} x \\ y \\ z \end{pmatrix}_1$$

$$\begin{pmatrix} -x \\ y \\ -z+1/2 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 1/2 \end{pmatrix}$$

Result of Sym. Op no (2) You always start with atom no. (1) x, y, z

-x: The linear function no 2 of (x,y,z) always results in -x

-x = -1 x + 0 y + 0 z First row of symmetry matrix

Not a scew axis

Translation NOT parallel to rotation axis

(2) 2 0, y, ¼

Determinant, Trace of W gives type
Solution to $\vec{r} = \boldsymbol{W}\vec{r}$ Give points on axis/plane